One-dimensional kinetic Ising model with nonuniform coupling constants

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Abstract

A nonuniform extension of the Glauber model on a one-dimensional lattice with boundaries is investigated. Based on detailed balance, reaction rates are proposed for the system. The static behavior of the system is investigated. It is shown that there are cases where the system exhibits a static phase transition, which is a change of behavior of the static profile of the expectation values of the spins near end points.

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1 Introduction

The Glauber dynamics was originally proposed to study the relaxation of the Ising model near equilibrium states. It is a simple non-equilibrium model of interacting spins with spin-flip dynamics. It is also known that there is a relation between the kinetic Ising model at zero temperature and the diffusion annihilation model in one dimension. There is an equivalence between domain walls in the Ising model and particles in the diffusion annihilation model. Kinetic generalizations of the Ising model, for example the Glauber model or the Kawasaki model, are phenomenological models and have been extensively studied [1–6]. Combination of the Glauber and the Kawasaki dynamics has been also considered [7–9]. Most studies are focused on completely uniform lattices with site-independent rates. Among the simplest generalizations beyond a completely uniform system is a lattice with alternating rates. In [10–12], the steady state configurational probabilities of an Ising spin chain driven out of equilibrium by a coupling to two heat baths has been investigated. An example is a one-dimensional Ising model on a ring, in which the evolution is according to a generalization of Glauber rates, such that spins at even (odd) lattice sites experience a temperature T_e (T_o). In this model the detailed balance is violated. The response function to an infinitesimal magnetic field for the Ising-Glauber model with arbitrary exchange couplings has been studied in [13]. Other generalizations of the Glauber model consist of, for example, alternating-isotopic chains and alternating-bound chains ([14] for example).

In [15], an asymmetric generalization of the zero-temperature Glauber model on a lattice with boundaries was introduced. There it was shown that in the thermodynamic limit, when the lattice becomes infinite, the system shows two kinds of phase transitions. One of these is a static phase transition, the other a dynamic one. The static phase transition is controlled by the reaction rates, and is a discontinuous change of the behavior of the derivative of the stationary magnetization at the end points, with respect to the reaction rates. The dynamic phase transition is controlled by the spin flip rates of the particles at the end points, and is a discontinuous change of the relaxation time towards the stationary configuration. Other phase transitions induced by boundary conditions have also been studied ([16–18] for example). Another generalization of the Glauber model was introduced in [19]. In this generalization, the processes are the same as those of the ordinary Glauber model, but the rates depend on three free parameters, rather than one free parameter in the ordinary Glauber model. Finally, this model was further generalized to the case where the number of interacting sites is more than three and the number of states at each site is more than two. This model too violates detailed balance.

In the present paper an Ising model on a nonuniform lattice with boundaries is investigated. Detailed balance is used to propose reaction rates for the system. Based on this, the evolution of the expectation values of spins is obtained. The time-independent solution to this equation is studied. This solution satisfies a homogeneous difference equation of the second order in the bulk, the solution to which can be expressed in terms of a transfer matrix. The reactions at the

boundaries impose nonhomogeneous (but at most linear) boundary conditions on this solution, which could be used to fix the constants appeared in the static solution. While it is true that the ordinary Ising model does not exhibit any phase transition in finite temperature (the expectation values of the spins vanish if there is no external magnetic field), this is not necessarily the case for the model studied here. The expectation values do not vanish as a result of inhomogeneous boundary conditions. It is shown that in the thermodynamic limit (when the size of the lattice tends to infinity) different phases could occur for this system, according to whether the eigenvalues of the transfer matrix are less than or larger than one. While this transition (or even the existence of nonzero static solutions) is invoked by the presence of inhomogeneous boundary conditions, the detailed form of the boundary conditions affects only the coefficients of the eigenvectors of the transition matrix in the static solution. So the detailed form of the boundary conditions do not affect the static phase portrait of the system. A closed form is obtained for this transfer matrix, and some examples are discussed, specially one example in which a phase transition is seen.

The scheme of the paper is as follows. In section 2, the model is introduced, the rates are determined using the detailed balance criterion, and the evolution equation for the spin expectation values is obtained. In section 3, the time-independent solution is studied, and the corresponding phase portrait is investigated. In section 4, some examples are studied in more detail, specially one example which exhibits a static phase transition. Section 5 is devoted to the concluding remarks.

2 One-dimensional Ising model with nonuniform coupling constants

Consider a one-dimensional lattice with $(L+1)$ sites, labeled from 0 to L. At each site, there is a spin variable, s_i, which could be $+1$ for spin up ($\uparrow$), or -1 for spin down ($\downarrow$). These spins in the bulk (s_i's with $0 < i < L$) interact according to the Ising Hamiltonian,

$$\mathcal{H} = -\sum_{\alpha} J_\alpha \, s_{\alpha-\mu} \, s_{\alpha+\mu}, \tag{1}$$

where J_α is the coupling constant in the link α, and

$$\mu := \frac{1}{2}. \tag{2}$$

The link α links the sites $\alpha - \mu$ and $\alpha + \mu$, so that $\alpha \pm \mu$ are integers, and α runs from μ up to $(L - \mu)$.

The usual Glauber model gives the dynamics of the Ising model with uniform coupling constants (J_α independent of α, and denoted by J) such that the rate of a spin flip is determined through its interaction with its two neighboring sites

and a heat bath at temperature T. A spin is flipped with the following rates.

$$\begin{aligned}
&\uparrow\uparrow\uparrow\,\to\,\uparrow\downarrow\uparrow \quad \text{and} \quad \downarrow\downarrow\downarrow\,\to\,\downarrow\uparrow\downarrow \quad \text{with rate} \quad 1-\tanh(2\,K),\\
&\uparrow\downarrow\uparrow\,\to\,\uparrow\uparrow\uparrow \quad \text{and} \quad \downarrow\uparrow\downarrow\,\to\,\downarrow\downarrow\downarrow \quad \text{with rate} \quad 1+\tanh(2\,K),\\
&\uparrow\uparrow\downarrow\,\rightleftharpoons\,\uparrow\downarrow\downarrow \quad \text{and} \quad \downarrow\downarrow\uparrow\,\rightleftharpoons\,\downarrow\uparrow\uparrow \quad \text{with rate} \quad 1,
\end{aligned} \tag{3}$$

where

$$K := \frac{J}{k_{\mathrm{B}}\,T}, \tag{4}$$

and k_{B} is the Boltzmann's constant. As it is seen, similar to the Ising model, the Glauber model has left-right and up-down symmetries. The Glauber model has also a particle reaction-diffusion interpretation. One considers a link with different spins at its sites (a domain wall) a particle ($\bullet$), and a link with same spins at its sites (no domain wall) a hole ($\circ$). Then the Glauber model turns into a reaction-diffusion model:

$$\begin{aligned}
&\circ\circ \to \bullet\bullet \quad \text{with rate} \quad 1-\tanh(2\,K),\\
&\bullet\bullet \to \circ\circ \quad \text{with rate} \quad 1+\tanh(2\,K),\\
&\bullet\circ \rightleftharpoons \circ\bullet \quad \text{with rate} \quad 1.
\end{aligned} \tag{5}$$

Consider the general case where the coupling constant is not uniform (and the interaction is not necessarily nearest neighbor). Assuming that in each step only one spin flips, detailed balance gives

$$\begin{aligned}
\frac{\omega(\cdots,s_j,\cdots\to\cdots,-s_j,\cdots)}{\omega(\cdots,-s_j,\cdots\to\cdots,s_j,\cdots)} &= \frac{\exp(\cdots+\sum_{i\ne j}K_{i\,j}\,s_i\,(-s_j)+\cdots)}{\exp(\cdots+\sum_{i\ne j}K_{i\,j}\,s_i\,s_j+\cdots)},\\
&= \frac{\exp(-h_j\,s_j)}{\exp(h_j\,s_j)},
\end{aligned} \tag{6}$$

where ω is the rate, $K_{i\,j}$ is defined like (4) but with $J_{i\,j}$ (the coupling between sites i and j) instead of J, and

$$h_j := \sum_{i\ne j} K_{i\,j}\,s_i. \tag{7}$$

As the value of s_i is either 1 or -1, any function of s_i is at most linear in s_i. One then arrives at

$$\exp(h_j\,s_j) = \cosh h_j + s_j\,\sinh h_j. \tag{8}$$

Using these, (6) gives

$$\frac{\omega(\cdots,s_j,\cdots\to\cdots,-s_j,\cdots)}{\omega(\cdots,-s_j,\cdots\to\cdots,s_j,\cdots)} = \frac{1-s_j\,\tanh h_j}{1+s_j\,\tanh h_j}, \tag{9}$$

or

$$\omega(\cdots,s_j,\cdots\to\cdots,-s_j,\cdots) = \Gamma_j\,(1-s_j\,\tanh h_j), \tag{10}$$

where Γ_j's are constants. In the simple case of nearest neighbor interaction, one has

$$J_{i\,j} = J_{i+\mu}\,\delta_{i,j-1} + J_{i-\mu}\,\delta_{i,j+1}, \tag{11}$$

so that (10) becomes

$$\omega(\cdots, s_j, \cdots \to \cdots, -s_j, \cdots) = \Gamma_j\,[1 - s_j\,\tanh(K_{j-\mu}\,s_{j-1} + K_{j+\mu}\,s_{j+1})], \tag{12}$$

So the spin at the site j flips according to following interactions with the indicated rates,

$$\begin{array}{llll}
\uparrow\uparrow\uparrow\to\uparrow\downarrow\uparrow & \text{and} & \downarrow\downarrow\downarrow\to\downarrow\uparrow\downarrow & \text{with rate}\quad 1-\tanh(K_{j-\mu}+K_{j+\mu}),\\
\uparrow\downarrow\uparrow\to\uparrow\uparrow\uparrow & \text{and} & \downarrow\uparrow\downarrow\to\downarrow\downarrow\downarrow & \text{with rate}\quad 1+\tanh(K_{j-\mu}+K_{j+\mu}),\\
\uparrow\uparrow\downarrow\to\uparrow\downarrow\downarrow & \text{and} & \downarrow\downarrow\uparrow\to\downarrow\uparrow\uparrow & \text{with rate}\quad 1-\tanh(K_{j-\mu}-K_{j+\mu}),\\
\downarrow\uparrow\uparrow\to\downarrow\downarrow\uparrow & \text{and} & \uparrow\downarrow\downarrow\to\uparrow\uparrow\downarrow & \text{with rate}\quad 1+\tanh(K_{j-\mu}-K_{j+\mu}),
\end{array} \tag{13}$$

where Γ_j's have been taken independent of j, and set to one by rescaling the time. As it could be expected, the left-right symmetry is violated, but the up-down symmetry is not. The particle reaction-diffusion picture turns into following reaction-diffusion model, which is not left-right symmetric, as expected.

$$\begin{array}{ll}
\circ\circ\to\bullet\bullet & \text{with rate}\quad 1-\tanh(K_{j-\mu}+K_{j+\mu}),\\
\bullet\bullet\to\circ\circ & \text{with rate}\quad 1+\tanh(K_{j-\mu}+K_{j+\mu}),\\
\circ\bullet\to\bullet\circ & \text{with rate}\quad 1-\tanh(K_{j-\mu}-K_{j+\mu}),\\
\bullet\circ\to\circ\bullet & \text{with rate}\quad 1+\tanh(K_{j-\mu}-K_{j+\mu}).
\end{array} \tag{14}$$

The evolution equation for the expectation values of the spins in the bulk turns out to be

$$\begin{aligned}
\langle\dot{s}_j\rangle = &\ -2\,\langle s_j\rangle + [\tanh(K_{j-\mu}+K_{j+\mu}) + \tanh(K_{j-\mu}-K_{j+\mu})]\,\langle s_{j-1}\rangle\\
&+ [\tanh(K_{j-\mu}+K_{j+\mu}) - \tanh(K_{j-\mu}-K_{j+\mu})]\,\langle s_{j+1}\rangle, \quad 0<j<L.
\end{aligned} \tag{15}$$

One has to add two other equations governing the evolution of s_0 and s_L. These are of the form

$$\begin{aligned}
\langle\dot{s}_0\rangle &= a_{-1} + a_0\,\langle s_0\rangle + a_1\,\langle s_1\rangle,\\
\langle\dot{s}_L\rangle &= a_{L+1} + a_L\,\langle s_L\rangle + a_{L-1}\,\langle s_{L-1}\rangle,
\end{aligned} \tag{16}$$

where a_j's are constants.

3 The static solution

For the static solution ($\langle s \rangle_{\mathrm{st}}$), the left hand side of (15) vanishes and one obtains

$$\begin{aligned}\langle s_{j+1}\rangle_{\mathrm{st}} = &-\frac{\sinh(2\,K_{j-\mu})}{\sinh(2\,K_{j+\mu})}\,\langle s_{j-1}\rangle_{\mathrm{st}}\\ &+\frac{\cosh(2\,K_{j-\mu})+\cosh(2\,K_{j+\mu})}{\sinh(2\,K_{j+\mu})}\,\langle s_j\rangle_{\mathrm{st}},\quad 0<j<L,\end{aligned} \tag{17}$$

which can be written as following matrix form

$$X_{j+\mu} = D_j\, X_{j-\mu}, \tag{18}$$

where

$$X_\alpha := \begin{pmatrix}\langle s_{\alpha-\mu}\rangle_{\mathrm{st}}\\ \langle s_{\alpha+\mu}\rangle_{\mathrm{st}}\end{pmatrix}, \tag{19}$$

and

$$D_j := \begin{pmatrix} 0 & 1\\ -\dfrac{\sinh(2\,K_{j-\mu})}{\sinh(2\,K_{j+h})} & \dfrac{\cosh(2\,K_{j-\mu})+\cosh(2\,K_{j+\mu})}{\sinh(2\,K_{j+\mu})}\end{pmatrix}. \tag{20}$$

One can write D_j as

$$D_j := \Sigma_{j+\mu}\,\Delta_j\,\Sigma_{j-\mu}^{-1}, \tag{21}$$

where

$$\Sigma_\alpha := \begin{pmatrix}\cosh K_\alpha & \sinh K_\alpha\\ \sinh K_\alpha & \cosh K_\alpha\end{pmatrix}, \tag{22}$$

and

$$\Delta_j := \begin{pmatrix}\dfrac{\sinh K_{j-\mu}}{\cosh K_{j+\mu}} & 0\\ 0 & \dfrac{\cosh K_{j-\mu}}{\sinh K_{j+\mu}}\end{pmatrix}. \tag{23}$$

Using (18), one arrives at

$$X_\alpha = D_{\alpha,\beta}\,X_\beta, \tag{24}$$

where

$$D_{\alpha,\beta} := \Sigma_\alpha\,\Delta_{\alpha,\beta}\,\Sigma_\beta^{-1}, \tag{25}$$

$$\Delta_{\alpha,\beta} := \Delta_{\alpha-\mu}\cdots\Delta_{\beta+\mu}, \tag{26}$$

so that,

$$\Delta_{\alpha,\beta} := \begin{pmatrix}\mathrm{M}_{\alpha,\beta}\,\dfrac{\sinh K_\beta}{\cosh K_\alpha} & 0\\ 0 & \mathrm{M}_{\alpha,\beta}^{-1}\,\dfrac{\cosh K_\beta}{\sinh K_\alpha}\end{pmatrix}, \tag{27}$$

and

$$D_{\alpha,\beta} = \begin{pmatrix} \left(\mathrm{M}_{\alpha,\beta} - \dfrac{1}{\mathrm{M}_{\alpha,\beta}}\right) \sinh K_\beta \, \cosh K_\beta & \dfrac{\cosh^2 K_\beta}{\mathrm{M}_{\alpha,\beta}} - \mathrm{M}_{\alpha,\beta} \sinh^2 K_\beta \\ \left(\Lambda_{\alpha,\beta} - \dfrac{1}{\Lambda_{\alpha,\beta}}\right) \sinh K_\beta \, \cosh K_\beta & \dfrac{\cosh^2 K_\beta}{\Lambda_{\alpha,\beta}} - \Lambda_{\alpha,\beta} \sinh^2 K_\beta \end{pmatrix}, \tag{28}$$

where

$$\Lambda_{\alpha,\beta} := \tanh K_\alpha \cdots \tanh K_{\beta+1}, \tag{29}$$

$$\mathrm{M}_{\alpha,\beta} := \tanh K_{\alpha-1} \cdots \tanh K_{\beta+1}. \tag{30}$$

The boundary conditions (16) are

$$\begin{aligned} A_\mu \, X_\mu &= -a_{-1}, \\ A_{L-\mu} \, X_{L-\mu} &= -a_{L+1}, \end{aligned} \tag{31}$$

where

$$A_\alpha := \begin{pmatrix} a_{\alpha-\mu} & a_{\alpha+\mu} \end{pmatrix}. \tag{32}$$

The steady state profile near the end-site 0 is determined by the eigenvalues of the matrix $D_{\alpha,\mu}$, where α is some site far from the ends. One has

$$\begin{aligned} X_\alpha &= X_\alpha^a \, \mathbf{f}_a, \\ X_\mu &= X_\mu^a \, \mathbf{f}_a, \end{aligned} \tag{33}$$

where $\mathbf{f}_a$ is the eigenvector of $D_{\alpha,\mu}$ corresponding to the eigenvalue λ^a, and X_α^a's and X_μ^a's are the coefficients of expansions of X_α and X_μ in terms of the eigenvectors. It is seen that

$$X_\alpha^a = \lambda^a \, X_\mu^a. \tag{34}$$

While the exact values of these coefficients are determined by the boundary conditions (31), one can say whether in the thermodynamic limit these coefficients vanish or not, without referring to the exact from of the boundary conditions.

In the thermodynamic limit, corresponding to each eigenvalue, two cases may occur.

i The eigenvalue λ^a tends to infinity. In this case X_μ^a tends to zero.

ii The eigenvalue λ^a tends to zero or a finite number. In this case X_μ^a is generally nonzero.

Obviously, similar cases occur at the other end point. It is seen that this behavior (some eigenvectors missing or not in the solution corresponding to the end points) at one of the end points is independent of the analog behavior at the other end.

4 Some examples

Consider some special cases.

1 Constant coupling:

$$K_\alpha = K. \tag{35}$$

In this case the relation of $D_{\alpha,\beta}$ with $\Delta_{\alpha,\beta}$ is a similarity transformation. So the eigenvalues $D_{\alpha,\beta}$ are the diagonal elements of $\Delta_{\alpha,\beta}$, which are

$$\begin{aligned} \lambda^1 &= \tanh^{\alpha-\mu} K, \\ \lambda^2 &= \coth^{\alpha-\mu} K, \end{aligned} \tag{36}$$

showing that one of the eigenvalues is larger and the other is smaller than one. So only one of the eigenvectors enters X_μ. This is regardless of the value of K. So there is no static phase transition, as it was seen in the case of ordinary (symmetric) Glauber model, [15].

2 Periodic coupling:

$$K_{\alpha+m} = K_\alpha. \tag{37}$$

In this case the behavior of the eigenvalues of $D_{\alpha,\mu}$ is determined by the eigenvalues of $D_{\alpha+m,\alpha}$, which are $\Lambda_{\alpha+m,\alpha}$ and $\Lambda^{-1}_{\alpha+m,\alpha}$. This shows that one of the eigenvalues is greater than one and the other is less than one. So the situation is similar to that of constant coupling.

3 Defects in the lattice: No new phenomena is seen, as long as the defects are localized, i.e. they are for from the end points. So if there is a lattice that has some defects but otherwise is uniform, the static behavior near the end points is similar to that of a uniform lattice.

4 A lattice with different behavior at different end points: The behaviors of the static solution near the two ends are independent of each other, provided the behavior change occurs far from the end points. So all the phenomena seen in previous special cases can be seen at each end point, independent of the other end point.

5 A lattice with different signs of coupling constants: One can define the new variables s' and couplings K as

$$s'_j := [\mathrm{sgn}(K_\mu)\cdots \mathrm{sgn}(K_{j-\mu})]\, s_j, \tag{38}$$

$$K'_\alpha := |K_\alpha| \tag{39}$$

where sgn is the sign function, and investigate the system in terms of these. So nothing new happens.

6 A lattice with increasing coupling constants (increasing towards an end point): Suppose that K_α is an increasing function of α, so that

$$\lim_{\alpha\to\infty} K_\alpha = \infty, \tag{40}$$

$$\lim_{\alpha\to\infty} \Lambda_{\alpha,\beta} = \Lambda, \tag{41}$$

where Λ is neither zero nor infinity. Using (29), it is seen that (41) implies

$$\lim_{\alpha\to\infty} \tanh K_\alpha = 1, \tag{42}$$

which is equivalent to (40). The criterion (41) itself, is equivalent to

$$\lim_{\alpha\to\infty} [\exp(-2\,K_{\beta+1}) + \cdots + \exp(-2\,K_\alpha)] = \ell, \tag{43}$$

where ℓ is finite. Assuming that this is the case, it is seen that $D_{\alpha,\beta}$ tends to a finite matrix D, where

$$D = \begin{pmatrix} \left(\Lambda - \dfrac{1}{\Lambda}\right) \sinh K_\beta\,\cosh K_\beta & \dfrac{\cosh^2 K_\beta}{\Lambda} - \Lambda\,\sinh^2 K_\beta \\ \left(\Lambda - \dfrac{1}{\Lambda}\right) \sinh K_\beta\,\cosh K_\beta & \dfrac{\cosh^2 K_\beta}{\Lambda} - \Lambda\,\sinh^2 K_\beta \end{pmatrix}. \tag{44}$$

So in this case both of the eigenvectors remain in X_μ.

The last case shows that there is a static phase transition. In one phase only one eigenvector remains in X_μ, while in the other phase both eigenvectors remain.

5 Concluding remarks

An Ising model with nonuniform coupling constants on a one-dimensional lattice with boundaries was studied. Based on detailed balance, the evolution of this model was investigated, from which an equation for the static solution was obtained. While it is known that ordinary one-dimensional Ising model does not exhibit any phase transition at nonzero temperatures, here the inhomogeneity at the boundary conditions does permit such a phase transition, while the exact form of the boundary conditions do not enter the static phase transition studied here. The static phase picture of the system was studied in general, and some examples were given including one exhibiting a static phase transition.

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